Estimation of Properties of Pure Components Using Improved Group-Contribution[+] (GC[+]) Based Models and Uncertainty Analysis

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Physical and thermodynamic properties of pure components are needed to carry out tasks such as process design and computer aided molecular/mixture design among others. The experimental values of properties of many important pure components have not been measured due to many reasons, and hence they must be estimated. Predictive methods such as the group-contribution[+] (GC[+]) method (combined group-contribution (GC) method and atom connectivity index (CI) method) are generally suitable to estimate the needed property values. For assessing the quality and reliability of the selected property prediction method, an engineer needs to know the uncertainties in the estimated property values obtained from that method. With this information, the engineer can then perform better- informed design calculations by taking into account these uncertainties. Hence, given the importance of reliable estimation of properties and uncertainties in the property estimates in the engineering calculations, this work aims to revise and improve GC[+] method based estimation of properties as well as to estimate the confidence intervals of estimated property values. To this end, a systematic methodology for property modeling and uncertainty analysis, in general, is developed and used. In total 21 properties of pure components, which include normal boiling point, critical constants, normal melting point among others have been analysed. The statistical analysis of the model performance for these properties is highlighted through several illustrative examples. Important issues related to property modeling such as thermodynamic consistency of the predicted properties (relation of normal boiling point versus critical temperature etc.) are analysed. The developed methodology is simple, yet sound and effective and provides not only the estimated property values using the GC[+] approach, but also the uncertainties in the estimated property values. This feature allows one to evaluate the effects of these uncertainties on the product-process design calculations thereby contributing to better-informed and reliable engineering solutions.